

Graduate Student Research Seminar

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Design kinetic parameters for improved resilience of materials under irradiation

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Abstract

High-entropy alloys (HEAs) have attracted significant attention in recent years due to their potentially improved radiation resistance compared to pure metals and terminal solid-solution alloys. However, among HEAs, there are millions of design possibilities considering all potential compositions. In this study, we develop criteria for designing HEAs with improved radiation resilience, accounting for defect properties to promote interstitial-vacancy recombination. First, we conduct rate theory calculations on defects, followed by Molecular Dynamics (MD) simulations on pure W and W-based multicomponent concentrated alloys. It is found that when the diffusion coefficients of single vacancies and interstitials become similar, and the effective migration energies of defects are at a minimum (maximum diffusivity), defect recombination becomes optimal, and the defect concentration is significantly reduced. This is supported by MD simulations indicating improved radiation resistance in V- and Cr-based alloys that satisfy the above-stated criteria. Furthermore, experimental observations also reinforce the proposed approach. This study sheds light on the design criteria for improved radiation resistance and helps material selection without the need for extensive experimental work.



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